

Electronic and Optoelectronic Properties of Semiconductor Structures

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Chapter 1

STRUCTURAL PROPERTIES OF SEMICONDUCTORS

1.1 INTRODUCTION

Semiconductors form the basis of most modern information processing devices. Electronic devices such as diodes, bipolar junction transistors, and field effect transistors drive modern electronic technology. Optoelectronic devices such as laser diodes, modulators, and detectors drive the optical networks. In addition to devices, semiconductor structures have provided the stages for exploring questions of fundamental physics. Quantum Hall effect and other phenomena associated with many-body effects and low dimensions have been studied in semiconductor structures.

It is important to recognize that the ability to examine fundamental physics issues and to use semiconductors in state of the art device technologies depends critically on the purity and perfection of the semiconductor crystal. Semiconductors are often associated with clean rooms and workers clad in “bunny suits” lest the tiniest stray particle get loose and latch onto the wafer being processed. Indeed, semiconductor structures can operate at their potential only if they can be grown with a high degree of crystallinity and if impurities and defects can be controlled. For high structural quality it is essential that a high quality substrate be available. This requires growth of bulk crystals which are then sliced and polished to allow epitaxial growth of thin semiconductor regions including heterostructures.

In this chapter we start with a brief discussion of the important bulk and epitaxial crystal growth techniques. We then discuss the important semiconductor crystal structures. We also discuss strained lattice structures and the strain tensor for such crystals. Strained epitaxy and its resultant consequences are now widely exploited in

semiconductor physics and it is important to examine how epitaxial growth causes distortions in the crystal lattice.

1.2 CRYSTAL GROWTH

1.2.1 Bulk Crystal Growth

Semiconductor technology depends critically upon the availability of high quality substrates with as large a diameter as possible. Bulk crystal growth techniques are used mainly to produce substrates on which devices are eventually fabricated. While for some semiconductors like Si and GaAs (to some extent for InP) the bulk crystal growth techniques are highly matured; for most other semiconductors it is difficult to obtain high quality, large area substrates. Several semiconductor technologies are dependent on substrates that are not ideal. For example, the nitrides GaN, AlN, InN are grown on SiC or sapphire substrates, since there is no reliable GaN substrate. The aim of the bulk crystal growth techniques is to produce single crystal boules with as large a diameter as possible and with as few defects as possible. In Si the boule diameters have reached 30 cm with boule lengths approaching 100 cm. Large size substrates ensure low cost device production.

For the growth of boules from which substrates are obtained, one starts out with a purified form of the elements that are to make up the crystal. One important technique that is used is the Czochralski (CZ) technique. In the Czochralski technique shown in Fig. 1.1, the melt of the charge (i.e., the high quality polycrystalline material) is held in a vertical crucible. The top surface of the melt is just barely above the melting temperature. A seed crystal is then lowered into the melt and slowly withdrawn. As the heat from the melt flows up the seed, the melt surface cools and the crystal begins to grow. The seed is rotated about its axis to produce a roughly circular cross-section crystal. The rotation inhibits the natural tendency of the crystal to grow along certain orientations to produce a faceted crystal.

The CZ technique is widely employed for Si, GaAs, and InP and produces long ingots (boules) with very good circular cross-section. For Si up to 100 kg ingots can be obtained. In the case of GaAs and InP the CZ technique has to face problems arising from the very high pressures of As and P at the melting temperature of the compounds. Not only does the chamber have to withstand such pressures, also the As and P leave the melt and condense on the sidewalls. To avoid the second problem one seals the melt by covering it with a molten layer of a second material (e.g., boron oxide) which floats on the surface. The technique is then referred to as liquid encapsulated Czochralski, or the LEC technique.

A second bulk crystal growth technique involves a charge of material loaded in a quartz container. The charge may be composed of either high quality polycrystalline material or carefully measured quantities of elements which make up a compound crystal. The container called a “boat” is heated till the charge melts and wets the seed crystal. The seed is then used to crystallize the melt by slowly lowering the boat temperature starting from the seed end. In the gradient-freeze approach the boat is pushed into a furnace (to melt the charge) and slowly pulled out. In the Bridgeman approach, the boat is kept stationary while the furnace temperature is temporally varied to form

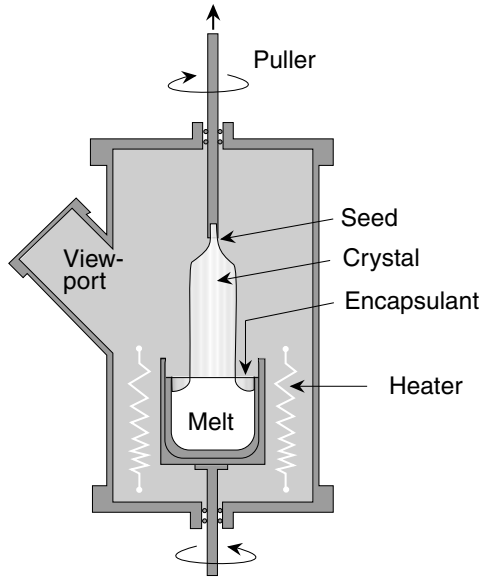


Figure 1.1: Schematic of Czochralski-style crystal grower used to produce substrate ingots. The approach is widely used for Si, GaAs and InP.

the crystal. The approaches are schematically shown in Fig. 1.2.

The easiest approach for the boat technique is to use a horizontal boat. However, the shape of the boule that is produced has a D-shaped form. To produce circular cross-sections vertical configurations have now been developed for GaAs and InP.

In addition to producing high purity bulk crystals, the techniques discussed above are also responsible for producing crystals with specified electrical properties. This may involve high resistivity materials along with *n*- or *p*-type materials. In Si it is difficult to produce high resistivity substrates by bulk crystal growth and resistivities are usually $<10^4 \Omega\text{-cm}$. However, in compound semiconductors carrier trapping impurities such as chromium and iron can be used to produce material with resistivities of $\sim 10^8 \Omega\text{-cm}$. The high resistivity or semi-insulating (SI) substrates are extremely useful in device isolation and for high speed devices. For *n*- or *p*-type doping carefully measured dopants are added in the melt.

1.2.2 Epitaxial Crystal Growth

Once bulk crystals are grown, they are sliced into substrates or wafers about $250 \mu\text{m}$ thick. These are polished and used for growth of epitaxial layers a few micrometers thick. All active devices are produced on these epitaxial layers. As a result the epitaxial growth techniques are very important. The epitaxial growth techniques have a very slow growth rate (as low as a monolayer per second for some techniques) which allow one to control very accurately the dimensions in the growth direction. In fact, in techniques like molecular beam epitaxy (MBE) and metal organic chemical vapor

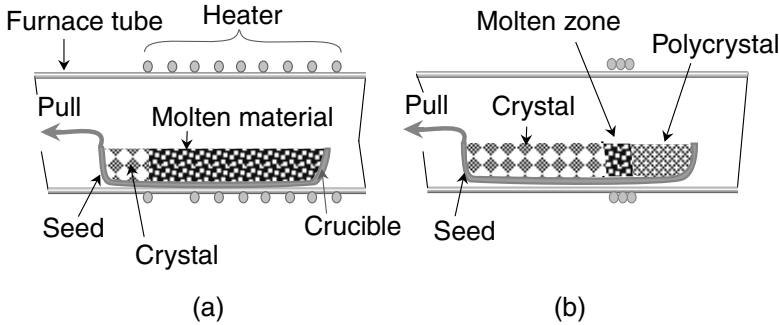


Figure 1.2: Crystal growing from the melt in a crucible: (a) solidification from one end of the melt (horizontal Bridgeman method); (b) melting and solidification in a moving zone.

deposition (MOCVD), one can achieve monolayer ($\sim 3 \text{ \AA}$) control in the growth direction. This level of control is essential for the variety of heterostructure devices that are being used in optoelectronics. The epitaxial techniques are also very useful for precise doping profiles that can be achieved. In fact, it may be argued that without the advances in epitaxial techniques that have occurred over the last two decades, most of the developments in semiconductor physics would not have occurred. Table 1.1 gives a brief view of the various epitaxial techniques used along with some of the advantages and disadvantages.

Liquid Phase Epitaxy (LPE)

LPE is a relatively simple epitaxial growth technique which was widely used until 1970s when it gradually gave way to approaches such as MBE and MOCVD. It is a less expensive technique (compared to MBE or MOCVD), but it offers less control in interface abruptness when growing heterostructures. LPE is still used for growth of crystals such as HgCdTe for long wavelength detectors and AlGaAs for double heterostructure lasers. As shown in Table 1.1, LPE is a close to equilibrium technique in which the substrate is placed in a quartz or a graphite boat and covered by a liquid of the crystal to be grown (see Fig. 1.3). The liquid may also contain dopants that are to be introduced into the crystal. LPE is often used for alloy growth where the growth follows the equilibrium solid-liquid phase diagram. By precise control of the liquid composition and temperature, the alloy composition can be controlled. Because LPE is a very close to equilibrium growth technique, it is difficult to grow alloy systems which are not miscible or even grow heterostructures with atomically abrupt interfaces. Nevertheless heterostructures where interface is graded over $10\text{-}20 \text{ \AA}$ can be grown by LPE by sliding the boat over successive “puddles” of different semiconductors. For many applications such interfaces are adequate and since LPE is a relatively inexpensive growth technique, it is used in many commercial applications.

Vapor Phase Epitaxy (VPE)

A large class of epitaxial techniques rely on delivering the components that form the crystal from a gaseous environment. If one has molecular species in a gaseous form with

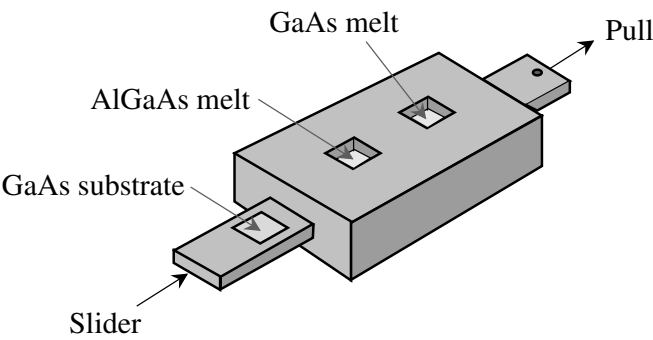


Figure 1.3: A schematic of the LPE growth of AlGaAs and GaAs. The slider moves the substrate, thus positioning itself to achieve contact with the different melts to grow heterostructures.

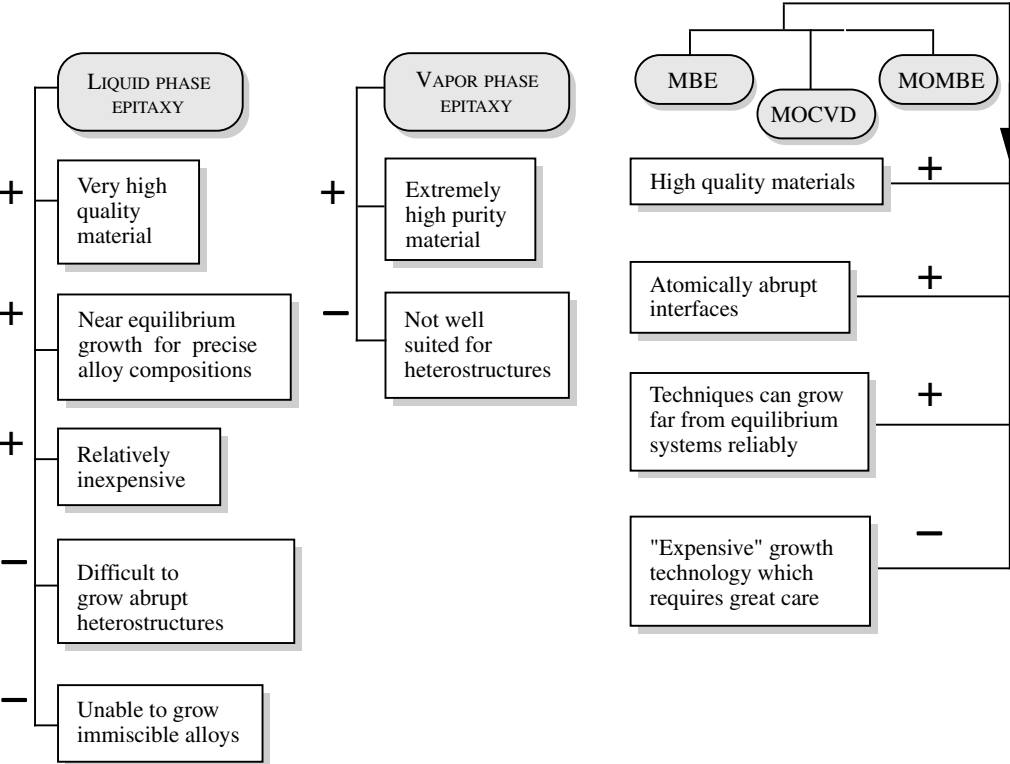


Table 1.1: A schematic of the various epitaxial crystal growth techniques and some of their positive and negative aspects.

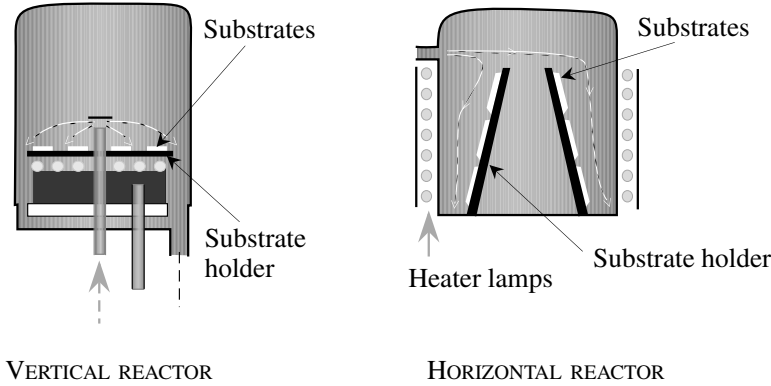


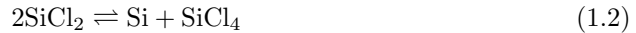
Figure 1.4: Reactors for VPE growth. The substrate temperature must be maintained uniformly over the area. This is achieved better by lamp heating. A pyrometer is used for temperature measurement.

partial pressure P , the rate at which molecules impinge upon a substrate is given by

$$F = \frac{P}{\sqrt{2\pi m k_B T}} \sim \frac{3.5 \times 10^{22} P(\text{torr})}{\sqrt{m(g)T(K)}} \text{mol./cm}^2\text{s} \quad (1.1)$$

where m is the molecular weight and T the cell temperature. For most crystals the surface density of atoms is $\sim 7 \times 10^{14} \text{ cm}^{-2}$. If the atoms or molecules impinging from the vapor can be deposited on the substrate in an ordered manner, epitaxial crystal growth can take place.

The VPE technique is used mainly for homoepitaxy and does not have the additional apparatus present in techniques such as MOCVD for precise heteroepitaxy. As an example of the technique, consider the VPE of Si. The Si containing reactant silane (SiH_4) or dichlorosilane (SiH_2Cl_2) or trichlorosilane (SiHCl_3) or silicon tetrachloride (SiCl_4) is diluted in hydrogen and introduced into a reactor in which heated substrates are placed as shown in Fig. 1.4. The silane pyrolysis to yield silicon while the chlorine containing gases react to give SiCl_2 , HCl and various other silicon-hydrogen-chlorine compounds. The reaction



then yields Si. Since HCl is also produced in the reaction, conditions must be tailored so that no etching of Si occurs by the HCl . Doping can be carried out by adding appropriate hydrides (phosphine, arsine, etc.,) to the reactants.

VPE can be used for other semiconductors as well by choosing different appropriate reactant gases. The reactants used are quite similar to those employed in the MOCVD technique discussed later.

Molecular Beam Epitaxy (MBE)

MBE is capable of controlling deposition of submonolayer coverage on a substrate and has become one of the most important epitaxial techniques. Almost every semiconductor

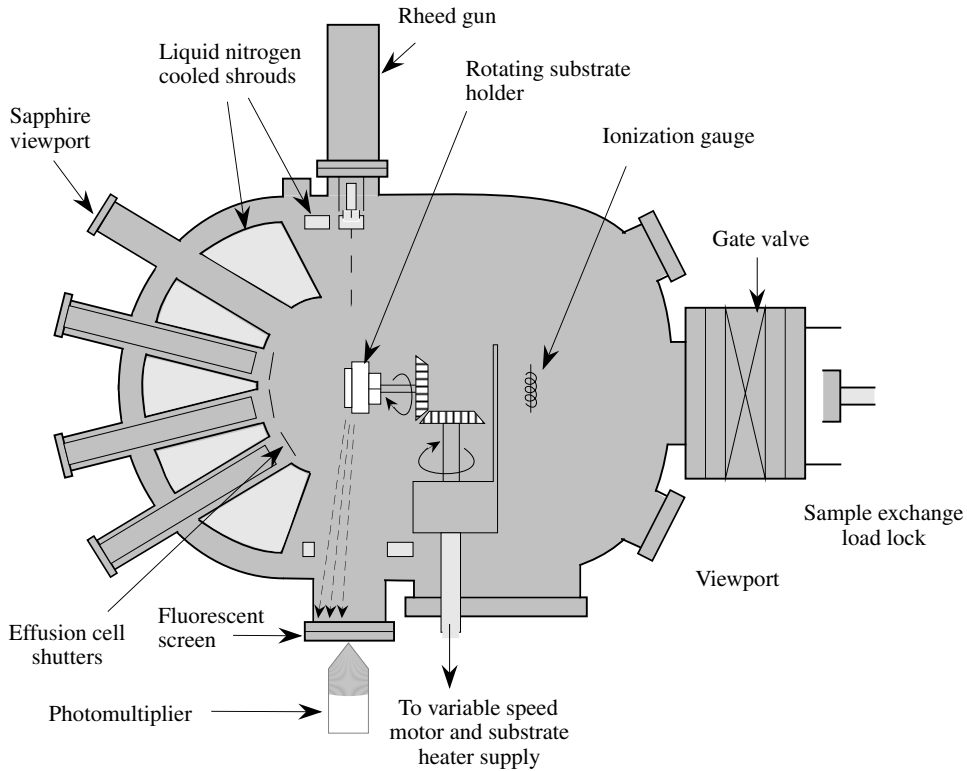


Figure 1.5: A schematic of the MBE growth system.

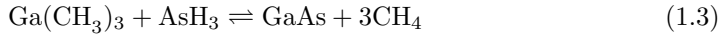
has been grown by this technique. MBE is a high vacuum technique ($\sim 10^{-11}$ torr vacuum when fully pumped down) in which crucibles containing a variety of elemental charges are placed in the growth chamber (Fig. 1.5). The elements contained in the crucibles make up the components of the crystal to be grown as well as the dopants that may be used. When a crucible is heated, atoms or molecules of the charge are evaporated and these travel in straight lines to impinge on a heated substrate.

The growth rate in MBE is ~ 1.0 monolayer per second and this slow rate coupled with shutters placed in front of the crucibles allow one to switch the composition of the growing crystal with monolayer control. Since no chemical reactions occur in MBE, the growth is the simplest of all epitaxial techniques and is quite controllable. However, since the growth involves high vacuum, leaks can be a major problem. The growth chamber walls are usually cooled by liquid N_2 to ensure high vacuum and to prevent atoms/molecules to come off from the chamber walls.

The low background pressure in MBE allows one to use electron beams to monitor the growing crystal. The reflection high energy electron diffraction (RHEED) techniques relies on electron diffraction to monitor both the quality of the growing substrate and the layer by layer growth mode.

Metal Organic Chemical Vapor Deposition (MOCVD)

Metal organic chemical vapor deposition (MOCVD) is another important growth technique widely used for heteroepitaxy. Like MBE, it is also capable of producing monolayer abrupt interfaces between semiconductors. A typical MOCVD system is shown in Fig. 1.6. Unlike in MBE, the gases that are used in MOCVD are not made of single elements, but are complex molecules which contain elements like Ga or As to form the crystal. Thus the growth depends upon the chemical reactions occurring at the heated substrate surface. For example, in the growth of GaAs one often uses triethyl gallium and arsine and the crystal growth depends upon the following reaction:



One advantage of the growth occurring via a chemical reaction is that one can use lateral temperature control to carry out local area growth. Laser assisted local area growth is also possible for some materials and can be used to produce new kinds of device structures. Such local area growth is difficult in MBE.

There are several varieties of MOCVD reactors. In the atmospheric MOCVD the growth chamber is essentially at atmospheric pressure. One needs a large amount of gases for growth in this case, although one does not have the problems associated with vacuum generation. In the low pressure MOCVD the growth chamber pressure is kept low. The growth rate is then slower as in the MBE case.

The use of the MOCVD equipment requires very serious safety precautions. The gases used are highly toxic and a great many safety features have to be incorporated to avoid any deadly accidents. Safety and environmental concerns are important issues in almost all semiconductor manufacturing since quite often one has to deal with toxic and hazardous materials.

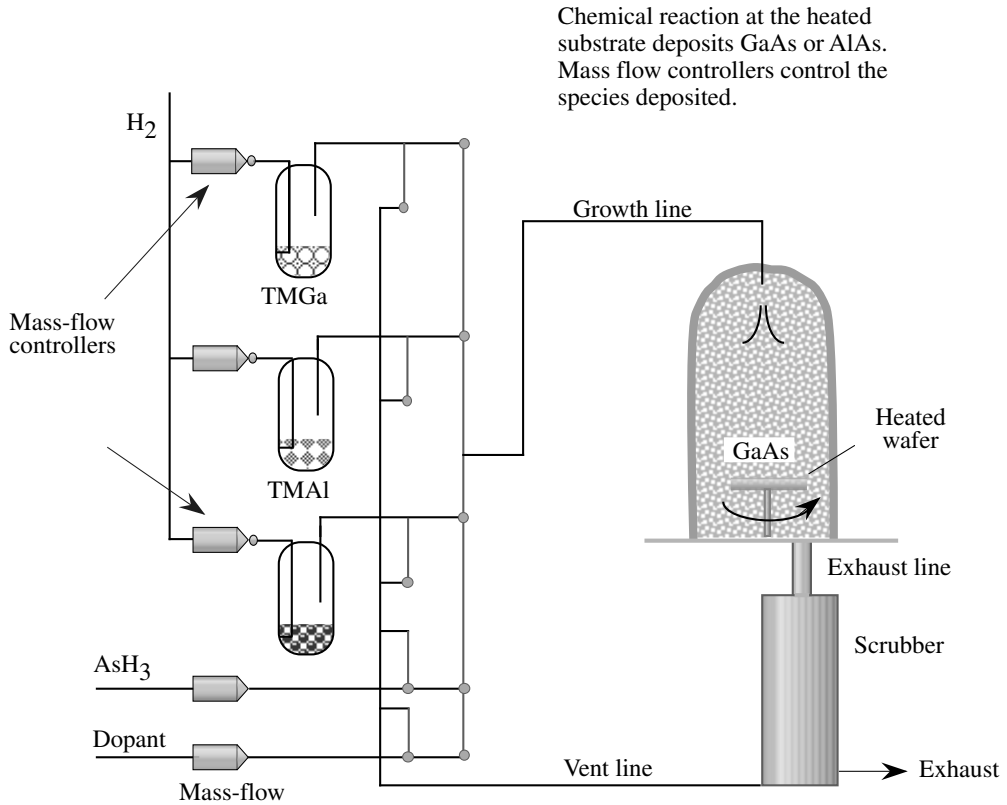
In addition to MBE and MOCVD one has hybrid epitaxial techniques often called MOMBE (metal organic MBE) which try to combine the best of MBE and MOCVD. In MBE one has to open the chamber to load the charge for the materials to be grown while this is avoided in MOCVD where gas bottles can be easily replaced from outside. Additionally, in MBE one has occasional spitting of material in which small clumps of atoms are evaporated off on to the substrate. This is avoided in MOCVD and MOMBE.

EXAMPLE 1.1 Consider the growth of GaAs by MBE. The Ga partial pressure in the growth chamber is 10^{-5} Torr, and the Ga cell temperature is 900 K. Calculate the flux of Ga atoms on the substrate. The surface density of Ga atoms on GaAs grown along (001) direction is $6.3 \times 10^{14} \text{ cm}^{-2}$. Calculate the growth rate if all of the impinging atoms stick to the substrate.

The mass of Ga atoms is 70 g/mole. The flux is (from Eqn. 1.1)

$$F = \frac{3.5 \times 10^{22} \times 10^{-5}}{\sqrt{70 \times 900}} = 5.27 \times 10^{14} \text{ atoms/cm}^2$$

Note that the surface density of Ga atoms on GaAs is $\sim 6.3 \times 10^{14} \text{ cm}^{-2}$. Thus, if all of the Ga atoms were to stick, the growth rate would be ~ 0.8 monolayer per second. This assumes that there is sufficient arsenic to provide As in the crystal. This is a typical growth rate for epitaxial films. It would take nearly 10 hours to grow a 10 μm film.



TMGa : Gallium containing organic compound
 TMAI : Aluminum containing organic compound
 AsH₃ : Arsenic containing compound

Figure 1.6: Schematic diagram of an MOCVD system employing alkyds (trimethyl gallium (TMGa) and trimethyl aluminum (TMAI) and metal hydride (arsine) material sources, with hydrogen as a carrier gas.

1.2.3 Epitaxial Regrowth

The spectacular growth of semiconductor microelectronics owes a great deal to the concept of the integrated circuit. The ability to fabricate transistors, resistors, inductors and capacitors on the same wafer is critical to the low cost and high reliability we have come to expect from microelectronics. It is natural to expect similar dividends from the concept of the optoelectronic integrated circuit (OEIC). In the OEIC, the optoelectronic device (the laser or detector or modulator) would be integrated on the same wafer with an amplifier or logic gates.

One of the key issues in OEICs involves etching and regrowth. As we will see

later, the optoelectronic devices have a structure that is usually not compatible with the structure of an electronic device. The optimum layout then involves growing one of the device structures epitaxially and then masking the region to be used as, say, the optoelectronic device and etching away the epitaxial region. Next a regrowth is done to grow the electronic device with a different structure. The process is shown schematically in Fig. 1.7. While this process looks simple conceptually, there are serious problems associated with etching and regrowth.

A critical issue in the epitaxial growth of a semiconductor layer is the quality of the semiconductor-vacuum interface. This semiconductor surface must be “clean,” i.e., there should be no impurity layers (e.g., an oxide layer) on the surface. Even if a fraction of a monolayer of the surface atoms have impurities bonded to them, the quality of the epitaxial layer suffers drastically. The growth may occur to produce microcrystalline regions separated by grain boundaries or may be amorphous in nature. In either case, the special properties arising from the crystalline nature of the material (to be discussed in the next chapter) are then lost.

The issue of surface cleanliness and surface reconstruction can be addressed when one is doing a single epitaxial growth. For example, a clean wafer can be loaded into the growth chamber and the remaining impurities on the surface can be removed by heating the substrate. The proper reconstruction (which can be monitored by RHEED) can be ensured by adjusting the substrate temperature and specy overpressure. Now consider the problems associated with etching after the first epitaxial growth has occurred. As the etching starts, foreign atoms or molecules are introduced on the wafer as the semiconductor is etched. The etching process is quite damaging and as it ends, the surface of the etched wafer is quite rough and damaged. In addition, in most growth techniques the wafer has to be physically moved from the high purity growth chamber to the etching system. During this transportation, the surface of the wafer may collect some “dirt.” During the etching process this “dirt” may not be etched off and may remain on the wafer. As a result of impurities and surface damage, when the second epitaxial layer is grown after etching, the quality of the layer suffers.

A great deal of processing research in OEICs focusses on improving the etching/regrowth process. So far the OEICs fabricated in various laboratories have performances barely approaching the performance of hybrid circuits. Clearly the problem of etching/regrowth is hampering the progress in OEIC technology.

It may be noted that the etching regrowth technology is also important in creating quantum wires and quantum dots which require lateral patterning of epitaxial layers.

1.3 CRYSTAL STRUCTURE

Essentially all high performance semiconductor devices are based on crystalline materials. there are some devices that use low cast amorphous or polycrystalline semiconductors, but their performance is quite poor. Crystals are made up of identical building blocks, the block being an atom or a group of atoms. While in “natural” crystals the crystalline symmetry is fixed by nature, new advances in crystal growth techniques are allowing scientists to produce artificial crystals with modified crystalline structure.

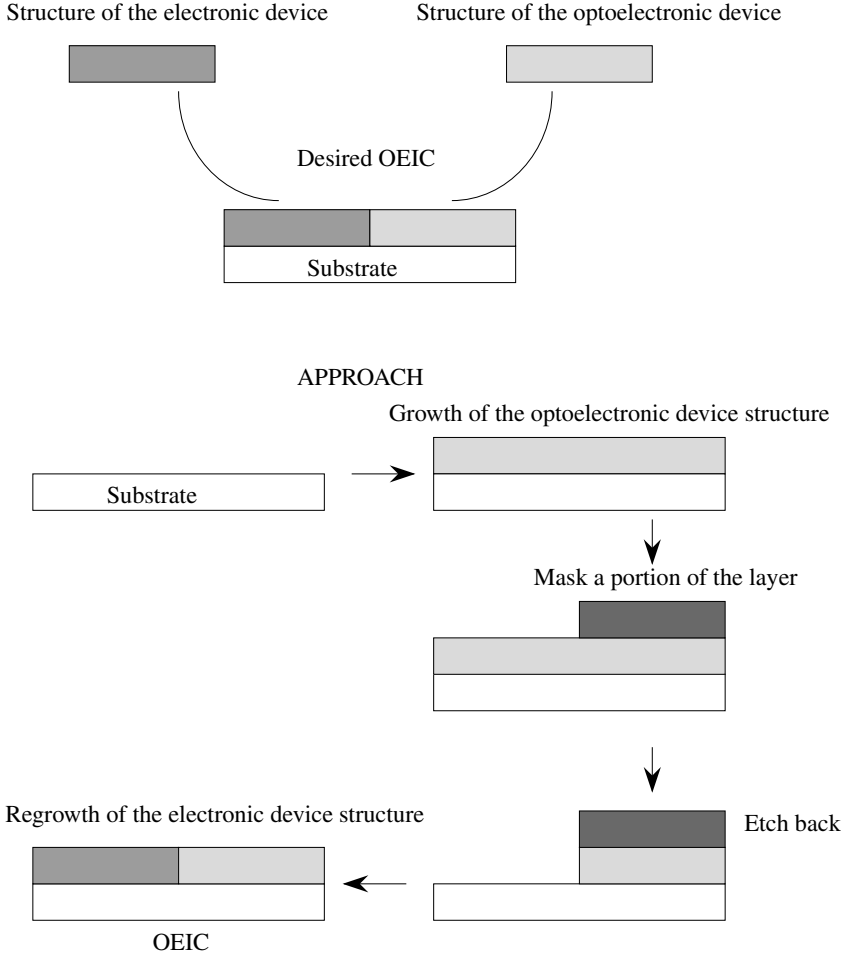


Figure 1.7: The importance of regrowth is clear when one examines the difference in the structure of electronic and optoelectronic devices. Etching and regrowth is essential for fabrication of optoelectronic integrated circuits (OEIC).

These advances depend upon being able to place atomic layers with exact precision and control during growth, leading to “superlattices”. To define the crystal structure, two important concepts are introduced. The *lattice* represents a set of points in space which form a periodic structure. Each point sees an exact similar environment. The lattice is by itself a mathematical abstraction. A building block of atoms called the *basis* is then attached to each lattice point yielding the crystal structure.

An important property of a lattice is the ability to define three vectors \mathbf{a}_1 , \mathbf{a}_2 , \mathbf{a}_3 , such that any lattice point \mathbf{R}' can be obtained from any other lattice point \mathbf{R} by a translation

$$\mathbf{R}' = \mathbf{R} + m_1\mathbf{a}_1 + m_2\mathbf{a}_2 + m_3\mathbf{a}_3 \quad (1.4)$$

where m_1, m_2, m_3 are integers. Such a lattice is called Bravais lattice. The entire lattice can be generated by choosing all possible combinations of the integers m_1, m_2, m_3 . The crystalline structure is now produced by attaching the basis to each of these lattice points.

$$\boxed{\text{lattice} + \text{basis} = \text{crystal structure}} \quad (1.5)$$

The translation vectors \mathbf{a}_1 , \mathbf{a}_2 , and \mathbf{a}_3 are called primitive if the volume of the cell formed by them is the smallest possible. There is no unique way to choose the primitive vectors. One choice is to pick

- \mathbf{a}_1 to be the shortest period of the lattice
- \mathbf{a}_2 to be the shortest period not parallel to \mathbf{a}_1
- \mathbf{a}_3 to be the shortest period not coplanar with \mathbf{a}_1 and \mathbf{a}_2

It is possible to define more than one set of primitive vectors for a given lattice, and often the choice depends upon convenience. The volume cell enclosed by the primitive vectors is called the *primitive unit cell*.

Because of the periodicity of a lattice, it is useful to define the symmetry of the structure. The symmetry is defined via a set of point group operations which involve a set of operations applied around a point. The operations involve rotation, reflection and inversion. The symmetry plays a very important role in the electronic properties of the crystals. For example, the inversion symmetry is extremely important and many physical properties of semiconductors are tied to the absence of this symmetry. As will be clear later, in the diamond structure (Si, Ge, C, etc.), inversion symmetry is present, while in the Zinc Blende structure (GaAs, AlAs, InAs, etc.), it is absent. Because of this lack of inversion symmetry, these semiconductors are piezoelectric, i.e., when they are strained an electric potential is developed across the opposite faces of the crystal. In crystals with inversion symmetry, where the two faces are identical, this is not possible.

1.3.1 Basic Lattice Types

The various kinds of lattice structures possible in nature are described by the symmetry group that describes their properties. Rotation is one of the important symmetry groups. Lattices can be found which have a rotation symmetry of $2\pi, \frac{2\pi}{2}, \frac{2\pi}{3}, \frac{2\pi}{4}, \frac{2\pi}{6}$. The rotation symmetries are denoted by 1, 2, 3, 4, and 6. No other rotation axes exist; e.g., $\frac{2\pi}{5}$ or $\frac{2\pi}{7}$ are not allowed because such a structure could not fill up an infinite space.

There are 14 types of lattices in 3D. These lattice classes are defined by the relationships between the primitive vectors a_1, a_2 , and a_3 , and the angles α, β , and γ between them. The general lattice is triclinic ($\alpha \neq \beta \neq \gamma, a_1 \neq a_2 \neq a_3$) and there are 13 special lattices. Table 1.2 provides the basic properties of these three dimensional lattices. We will focus on the cubic lattice which is the structure taken by all semiconductors.

There are 3 kinds of cubic lattices: simple cubic, body centered cubic, and face centered cubic.

System	Number of lattices	Restrictions on conventional cell axes and singles
Triclinic	1	$a_1 \neq a_2 \neq a_3$ $\alpha \neq \beta \neq \gamma$
Monoclinic	2	$a_1 \neq a_2 \neq a_3$ $\alpha = \gamma = 90^\circ \neq \beta$
Orthorhombic	4	$a_1 \neq a_2 \neq a_3$ $\alpha = \beta = \gamma = 90^\circ$
Tetragonal	2	$a_1 = a_2 \neq a_3$ $\alpha = \beta = \gamma = 90^\circ$
Cubic	3	$a_1 = a_2 = a_3$ $\alpha = \beta = \gamma = 90^\circ$
Trigonal	1	$a_1 = a_2 = a_3$ $\alpha = \beta = \gamma < 120^\circ, \neq 90^\circ$
Hexagonal	1	$a_1 = a_2 \neq a_3$ $\alpha = \beta = 90^\circ$ $\gamma = 120^\circ$

Table 1.2: The 14 Bravais lattices in 3-dimensional systems and their properties.

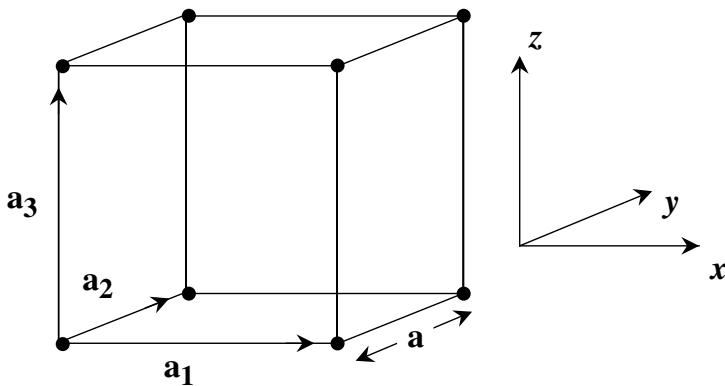


Figure 1.8: A simple cubic lattice showing the primitive vectors. The crystal is produced by repeating the cubic cell through space.

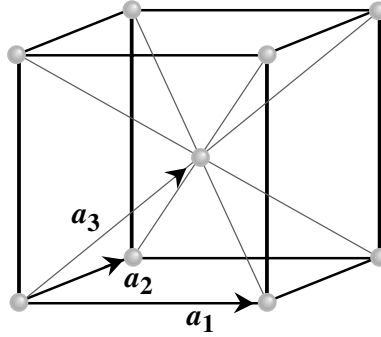


Figure 1.9: The body centered cubic lattice along with a choice of primitive vectors.

Simple cubic: The simple cubic lattice shown in Fig. 1.8 is generated by the primitive vectors

$$a\mathbf{x}, a\mathbf{y}, a\mathbf{z} \quad (1.6)$$

where the $\mathbf{x}, \mathbf{y}, \mathbf{z}$ are unit vectors.

Body-centered cubic: The bcc lattice shown in Fig. 1.9 can be generated from the simple cubic structure by placing a lattice point at the center of the cube. If $\hat{\mathbf{x}}, \hat{\mathbf{y}},$ and $\hat{\mathbf{z}}$ are three orthogonal unit vectors, then a set of primitive vectors for the body-centered cubic lattice could be

$$a_1 = a\hat{\mathbf{x}}, a_2 = a\hat{\mathbf{y}}, a_3 = \frac{a}{2}(\hat{\mathbf{x}} + \hat{\mathbf{y}} + \hat{\mathbf{z}}) \quad (1.7)$$

A more symmetric set for the bcc lattice is

$$a_1 = \frac{a}{2}(\hat{\mathbf{y}} + \hat{\mathbf{z}} - \hat{\mathbf{x}}), a_2 = \frac{a}{2}(\hat{\mathbf{z}} + \hat{\mathbf{x}} - \hat{\mathbf{y}}), a_3 = \frac{a}{2}(\hat{\mathbf{x}} + \hat{\mathbf{y}} - \hat{\mathbf{z}}) \quad (1.8)$$

Face Centered Cubic: Another equally important lattice for semiconductors is the *face-centered cubic* (fcc) Bravais lattice. To construct the face-centered cubic Bravais lattice add to the simple cubic lattice an additional point in the center of each square face (Fig. 1.10).

A symmetric set of primitive vectors for the face-centered cubic lattice (see Fig. 1.10) is

$$a_1 = \frac{a}{2}(\hat{\mathbf{y}} + \hat{\mathbf{z}}), a_2 = \frac{a}{2}(\hat{\mathbf{z}} + \hat{\mathbf{x}}), a_3 = \frac{a}{2}(\hat{\mathbf{x}} + \hat{\mathbf{y}}) \quad (1.9)$$

The face-centered cubic and body-centered cubic Bravais lattices are of great importance, since an enormous variety of solids crystallize in these forms with an atom (or ion) at each lattice site. Essentially all semiconductors of interest for electronics and optoelectronics have fcc structure.

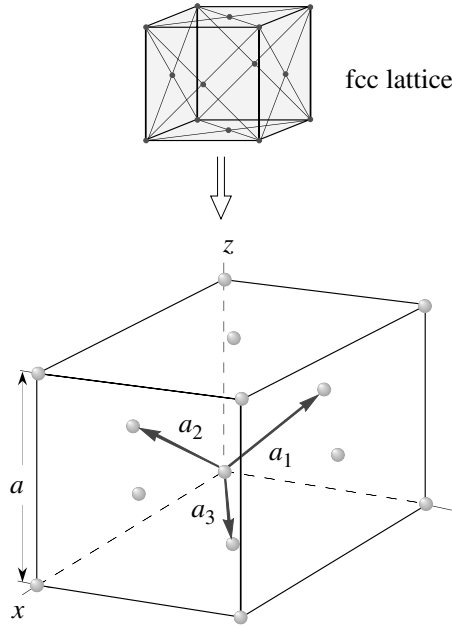


Figure 1.10: Primitive basis vectors for the face centered cubic lattice.

1.3.2 Basic Crystal Structures

Diamond and Zinc Blende Structures

Most semiconductors of interest for electronics and optoelectronics have an underlying fcc lattice. However, they have two atoms per basis. The coordinates of the two basis atoms are

$$(000) \text{ and } \left(\frac{a}{4}, \frac{a}{4}, \frac{a}{4}\right) \quad (1.10)$$

Since each atom lies on its own fcc lattice, such a two atom basis structure may be thought of as two inter-penetrating fcc lattices, one displaced from the other by a translation along a body diagonal direction $\left(\frac{a}{4}, \frac{a}{4}, \frac{a}{4}\right)$.

Figure 1.11 gives details of this important structure. If the two atoms of the basis are identical, the structure is called diamond. Semiconductors such as Si, Ge, C, etc., fall in this category. If the two atoms are different, the structure is called the Zinc Blende structure. Semiconductors such as GaAs, AlAs, CdS, etc., fall in this category. Semiconductors with diamond structure are often called elemental semiconductors, while the Zinc Blende semiconductors are called compound semiconductors. The compound semiconductors are also denoted by the position of the atoms in the periodic chart, e.g., GaAs, AlAs, InP are called III-V (three-five) semiconductors while CdS, HgTe, CdTe, etc., are called II-VI (two-six) semiconductors.

Hexagonal Close Pack Structure The hexagonal close pack (hcp) structure is an important lattice structure and many metals have this underlying lattice. Some

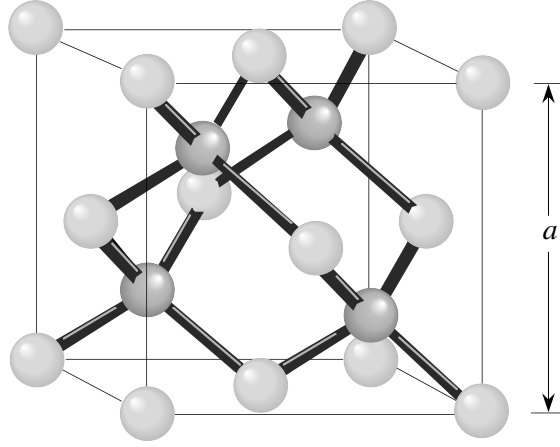


Figure 1.11: The zinc blende crystal structure. The structure consists of the interpenetrating fcc lattices, one displaced from the other by a distance $(\frac{a}{4}, \frac{a}{4}, \frac{a}{4})$ along the body diagonal. The underlying Bravais lattice is fcc with a two atom basis. The positions of the two atoms is (000) and $(\frac{a}{4}, \frac{a}{4}, \frac{a}{4})$.

semiconductors such as BN, AlN, GaN, SiC, etc., also have this underlying lattice (with a two-atom basis). The hcp structure is formed as shown in Fig. 1.12a. Imagine that a close-packed layer of spheres is formed. Each sphere touches six other spheres, leaving cavities, as shown. A second close-packed layer of spheres is placed on top of the first one so that the second layer sphere centers are in the cavities formed by the first layer. The third layer of close-packed spheres can now be placed so that center of the spheres do not fall on the center of the starting spheres (left side of Fig. 1.12a) or coincide with the centers of the starting spheres (right side of Fig. 1.12b). These two sequences, when repeated, produce the fcc and hcp lattices.

In Fig. 1.12b we show the detailed positions of the lattice points in the hcp lattice. The three lattice vectors are a_1 , a_2 , a_3 , as shown. The vector a_3 is denoted by c and the term c -axis refers to the orientation of a_3 . In an ideal structure, if $|a| = |a_1| = |a_2|$,

$$\frac{c}{a} = \sqrt{\frac{8}{3}} \quad (1.11)$$

In Table 1.3 we show the structural properties of some important materials. If two or more semiconductors are randomly mixed to produce an alloy, the lattice constant of the alloy is given by Vegard's law according to which the alloy lattice constant is the weighted mean of the lattice constants of the individual components.

1.3.3 Notation to Denote Planes and Points in a Lattice: Miller Indices

A simple scheme is used to describe lattice planes, directions and points. For a plane, we use the following procedure:

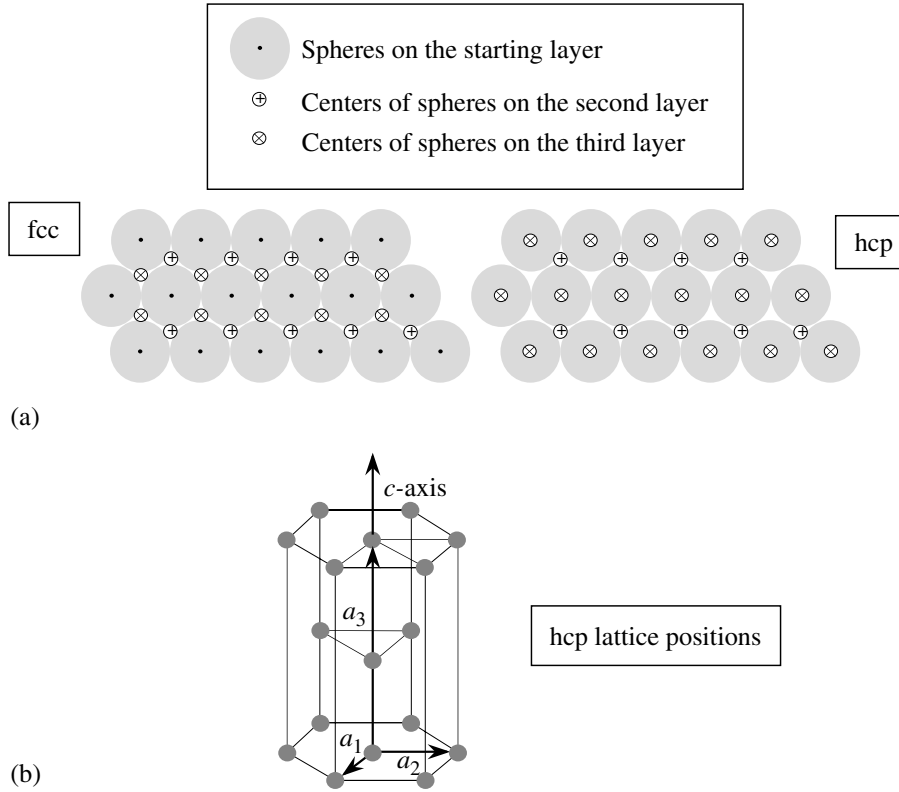


Figure 1.12: (a) A schematic of how the fcc and hcp lattices are formed by close packing of spheres. (b) Arrangement of lattice points on an hcp lattice.

- (1) Define the x , y , z axes (primitive vectors).
- (2) Take the intercepts of the plane along the axes in units of lattice constants.
- (3) Take the reciprocal of the intercepts and reduce them to the smallest integers.

The notation (hkl) denotes a family of parallel planes.

The notation $\{hkl\}$ denotes a family of equivalent planes.

To denote directions, we use the smallest set of integers having the same ratio as the direction cosines of the direction.

In a cubic system the Miller indices of a plane are the same as the direction perpendicular to the plane. The notation $[]$ is for a set of parallel directions; $\langle \rangle$ is for a set of equivalent direction. Fig. 1.13 shows some examples of the use of the Miller indices to define planes.

EXAMPLE 1.2 The lattice constant of silicon is 5.43 \AA . Calculate the number of silicon atoms in a cubic centimeter. Also calculate the number density of Ga atoms in GaAs which

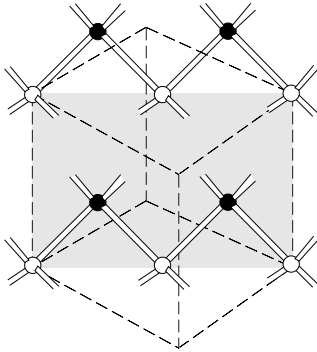
Material	Structure	Lattice Constant (Å)	Density (gm/cm ³)
C	Diamond	3.5668	3.5153
Si	Diamond	5.431	2.329
Ge	Diamond	5.658	5.323
GaAs	Zinc Blende	5.653	5.318
AlAs	Zinc Blende	5.660	3.760
InAs	Zinc Blende	6.058	5.667
GaN	Wurtzite	$a = 3.175; c = 5.158$	6.095
AlN	Wurtzite	$a = 3.111; c = 4.981$	3.255
SiC	Zinc Blende	4.360	3.166
Cd	hcp	$a = 2.98; c = 5.620$	8.65
Cr	bcc	2.88	7.19
Co	hcp	$a = 2.51; c = 4.07$	8.9
Au	fcc	4.08	19.3
Fe	bcc	2.87	7.86
Ag	fcc	4.09	10.5
Al	fcc	4.05	2.7
Cu	fcc	3.61	8.96

Table 1.3: Structure, lattice constant, and density of some materials at room temperature.

has a lattice constant of 5.65 Å.

Silicon has a diamond structure which is made up of the fcc lattice with two atoms on each lattice point. The fcc unit cube has a volume a^3 . The cube has eight lattice sites at the cube edges. However, each of these points is shared with eight other cubes. In addition, there are six lattice points on the cube face centers. Each of these points is shared by two adjacent cubes. Thus the number of lattice points per cube of volume a^3 are

$$N(a^3) = \frac{8}{8} + \frac{6}{2} = 4$$

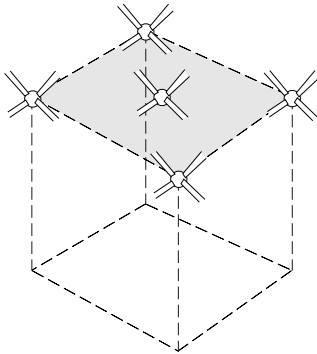


ATOMS ON THE (110) PLANE

Each atom has 4 bonds:

- 2 bonds in the (110) plane
- 1 bond connects each atom to adjacent (110) planes

⇒ Cleaving adjacent planes requires breaking 1 bond per atom

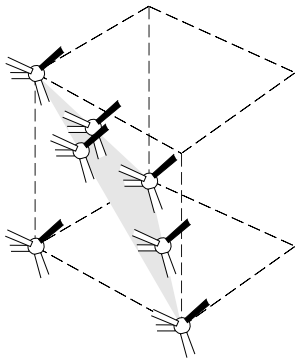


ATOMS ON THE (001) PLANE

2 bonds connect each atom to adjacent (001) plane

Atoms are either Ga or As in a GaAs crystal

⇒ Cleaving adjacent planes requires breaking 2 bonds per atom



ATOMS ON THE (111) PLANE

Could be either Ga or As

1 bond connecting an adjacent plane on one side

3 bonds connecting an adjacent plane on the other side

Figure 1.13: Some important planes in the cubic system along with their Miller indices. This figure also shows how many bonds connect adjacent planes. This number determines how easy or difficult it is to cleave the crystal along these planes.